ATOMIC TRANSFORMATION IN TETRAGONAL CuPt ALLOY UNDER UNIAXIAL TENSION AT LOW TEMPERATURE

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In the paper feature of atomic transformation was considered in CuPt alloy during dynamic deformation. Characteristics were studied for different stages: from primary tension to beginning of slip till crystal rupture. the transformation of atomic planes displacements and defects forming during tension has been studied. The investigation was revealed three main deformation processes at velocity 20 m/s and temperature 300 K, Quasi-elastic deformation, slipping and alloy fracture. Every stage is characterized by behavior of stored energy curve and some types of defects appearance. Vacancies, Frenkel pairs and interstitial atoms were found during first stage . Atomic displacement, dislocation, antiphase boundary and grain boundary forming were occurred during second stage. During third stage twins creation from grain boundaries has occurred.

Introduction

The scientific literature has paid much attention to the study of nanomaterials. Nowadays, there is a large variety of the unique properties of nano-objects which can be used in the design and development of new materials. Nanowires and nanotubes are determined in the groups of nanostructures and nanomaterials. Nanowires based on ordered alloys and intermetallic compounds are an interesting group of nanomaterials for their research. Major studies of metallic nanowires are devoted to the study of the influence of the configuration and structure of nanowires on the physical and mechanical properties. There are a number of publications on the mechanical properties of Ni nanowires in literature [1-5].

Mathematical model

The experiment was made on the calculated block of crystal simulating three-dimensional CuPt alloy. To calculate the dynamics of the atomic structure, the method of molecular dynamics using Morse pair potentials was used [6]:

$$\varphi_{KL}(r) = D_{KL}\beta_{KL}e^{-\alpha_{KL}r}\left[\beta_{KL}e^{-\alpha_{KL}r} - 2\right] \quad (1)$$

where α_{KL}, β_{KL}, D_{KL} - parameters defining the interaction of pairs of atoms of type K and L; r - the distance between the atoms.

The size of the calculated block of the nanowire made 10368 atoms that corresponded to the packing from 24 atoms along the side in the basis of a rectangular parallelepiped (4,2352 nm × 4,7809 nm) and 36 atoms in its height (6,9611 nm). Free boundary conditions were applied to the calculated block of the

crystal in directions <010> and <001> and rigid boundary conditions in direction <100>.

In the experiment process, the reserved energy per a separate atom was calculated at each stage of deformation in the dependence on time. The visualization of the three-dimensional atomic calculated block of crystal with possibility of turn and allocation of the atomic planes in the given directions has been made to observe the evolution of defect structure at the atomic level.

Results and discussions

For CuPt alloy with orientation axis of tension in the <001> the dependence of the stored energy of deformation of the crystal of time stretching. This graph is divided into four main stages of structural and energy transformations: the quasi-elastic deformation, plastic deformation, flow (necking) and fracture (Figure 1).

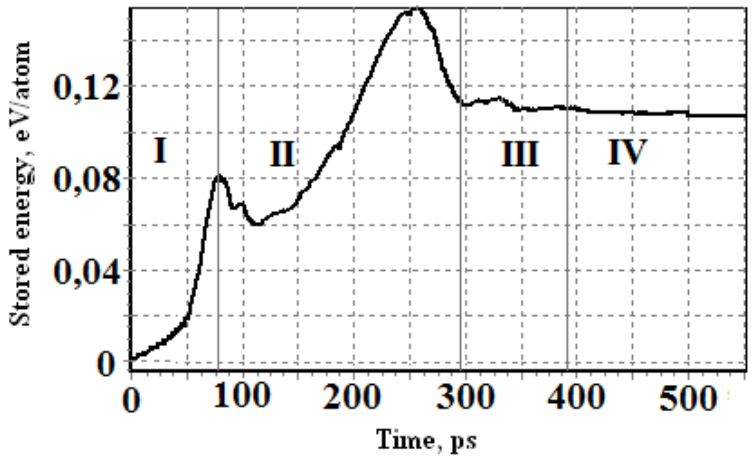

Fig.1. The change of the stored energy of CuPt alloy during the structural and energy transformations in the process of deformation

The initial stage — quasi-elastic deformation, when small displacements of atoms take place and the defects are not observed. In the given section of the graph, the stored energy according to a parabolic law. The first stage comes to the end at the point of energy bifurcation.

Consecutive splitting of the family of atomic planes in {001} into monatomic ones, was observed at the first stage due to the differences in the distances between the atomic layers in the directions <001> .

The described splitting of the planes family in {001} into monatomic planes takes place in the central part of the alloy more intensively (fig. 2). At the end of the first stage of splitting, the deformation of planes family in {001} was observed near rigid captures that led to the formation of the crack on the boundary of the section between absolutely rigid captures and the calculated block of the alloy. The significant atomic displacements were determined near the captures at the end of the first deformation stage. The tension at captures reached 12 GPa.

At the end of the second stage shows the place of formation of a "neck" Fig.3. In the third stage (early break) restructuring is primarily near the

"neck" (Fig. 4), which is reflected in the change of the schedule stored energy (Fig.1) at the site.

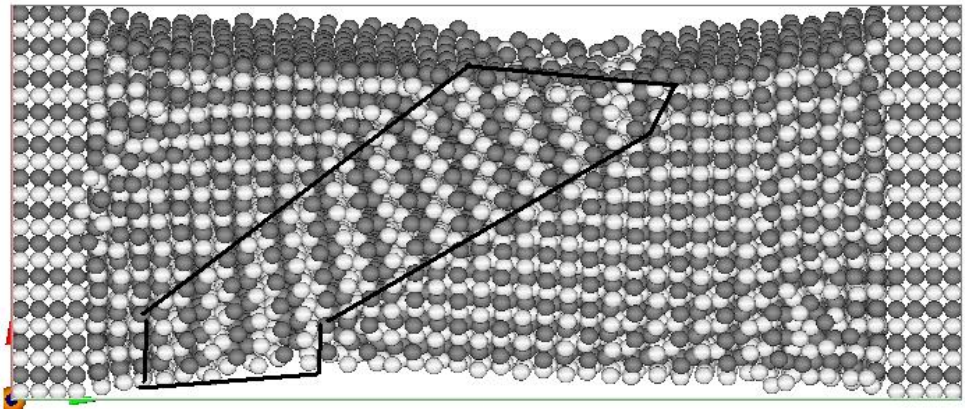

Fig. 2. end of the first stage of CuPt alloy, the formation of a domain in the central portion at 60 ps in the direction <001>

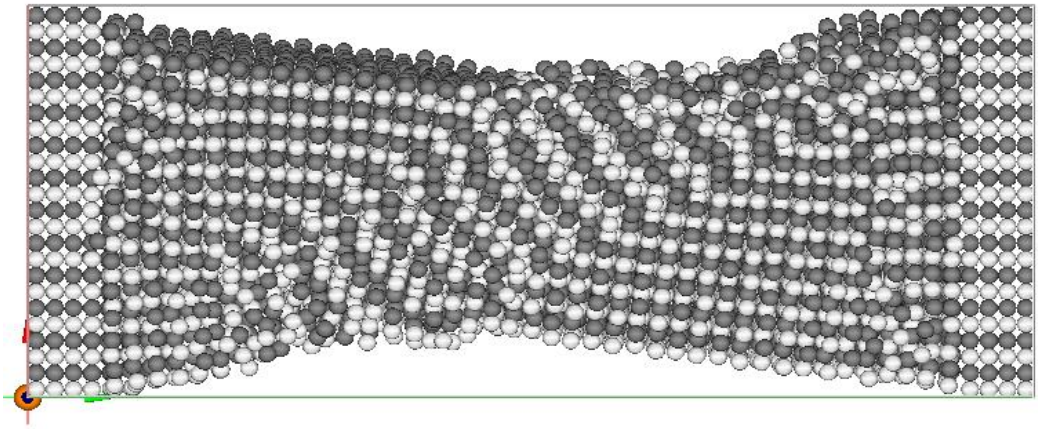

Fig.3. Atomic configuration of the second stage of CuPt alloy, at 100 ps deformation in the direction <001>

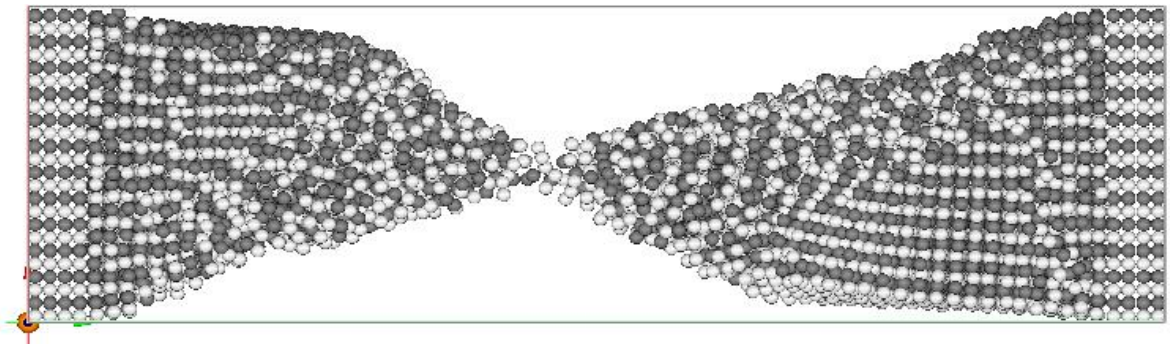

Fig.4. Atomic configuration of CuPt alloy, at 320 ps deformation in the direction <001>

It is shown that anisotropy of structure- energetic changes taking place in alloys depends on orientation of the alloy. In particular, the development of plastic deformation stages in the direction <001> occurs the formation of anti-phase boundaries and C-domains.

Conclusion

As a result of studies of structural and energy transformations during tensile deformation of CuPt alloys properties on the example of non-cubic symmetry of alloys at low temperature, identified four stages of structural and energy transformations: the quasi-elastic, plastic, flow and fracture.

1. The first stage of structural and energy transformations in the deformation process ends with formation sliding on the substructure of CuPt alloys. At the first stage of deformation, we can see rotation the central portion of nan-alloy and C-domain formation in the second stage of deformation.

2. It was found that the features of structural and energy transformations for non-cubic symmetry of alloys in the second stage of deformation affects the orientation of the axis of tension.

3. The neck area occur in the third stage of structural and energy transformations. Stored strain energy in that period varied only slightly.

4.The nature of the destruction of blocks corresponds to brittle fracture at low temperatures.

REFERENCES:

[1] M.M. Aish, M.D. Starostenkov, Effect of volume on the mechanical properties of nickel nanowire// Materials Physics and Mechanics, vol. 18, no. 1, (2013) pp. 53–62.

[2] M.D. Starostenkov, M.M. Aish, A.A. Sitnikov, S. A. Kotrechko, Deformation of different nickel nanowires at 300 K // Letters on Materials, V.3 is.3, (2013), P.180-183.

[3] Starostenkov M.D., Aish M.M. Effect of length and cross-sectional area on Ni3Fe alloy plasticity // Advanced Materials Research. (2014). V.1013. P. 242-248.

[4] MD Starostenkov, MM Aish, Molecular dynamic study for ultrathin Nickel nanowires at the same temperature, Materials Physics and Mechanics, (2014), vol. 21, no. 1, p. 1-7.

[5] M.D. Starostenkov, M.M. Aish, Feature of deformation and breaking of Ni nanowire // Letters on Materials, V.4 is.2, (2014), P.89-92.

[6] X. Yang, L. Liu, P. Zhai, Q. Zhang // Computational Materials Science 44 (2009) 1390.